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Functional properties of the charged domain walls and phase boundaries in the $BiFeO_3$ thin films and bulk ceramics

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In this contribution, we go deeper in understanding the local properties of the interfaces in BFO thin films and RE-BFO ceramics in order to build a comprehensive behavioral model that captures both local and macroscopic electromechanical properties in the same materials.

Bismuth ferrite (BFO) is a material possessing an unique set of properties such as large piezoelectric coefficients, abnormal photovoltaic effect and large values of photocurrents, coupling of spontaneous polarization and magnetic moment coexisting at room temperature [1]. BFO is a prime candidate lead-free electroceramic with wide sweeping potential as a multiferroic, piezoelectric and nanoelectronic material [2]. Rare-earth modified bismuth ferrites (RE-BFO) have enhanced magnetic [3] and electrical properties [4] as well as a simple chemistry, making them an excellent system for mapping the composition-structure-property evolution in BFO-based solid solutions.

The different interfaces exhibited in BFO: neutral and charged domain walls, phase and grain boundaries have an enhanced conductivity which play a specific role in the macroscopic material properties [5]. The strong relation between dielectric, piezoelectric properties of the material and the microscopic mechanism of the charge transfer across the interfaces was revealed in BFO ceramics [6,7].

In this contribution, we go deeper in understanding the local properties of the interfaces in BFO thin films and RE-BFO ceramics in order to build a comprehensive behavioral model that captures both local and macroscopic electromechanical properties in the same materials.

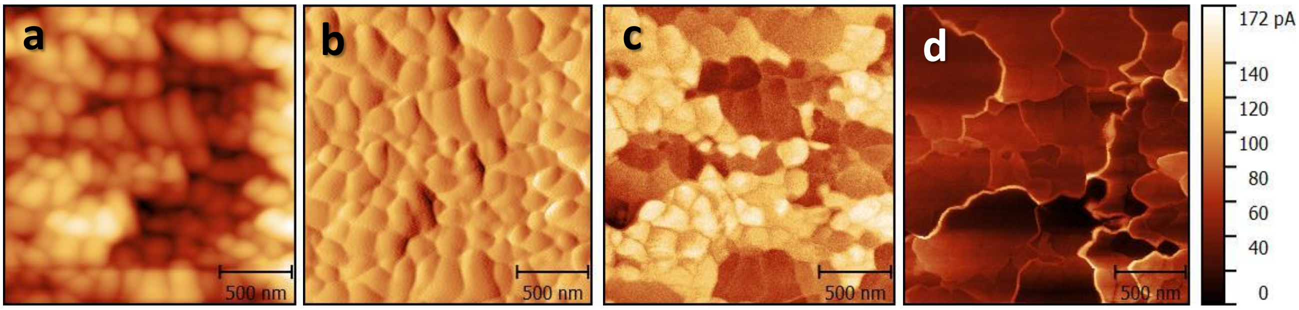

Figure 1. Correspondence between photoconductivity and domain structure in the BFO thin films: (a) topography, (b) differential topography, (c) vertical PFM phase, (d) photo-current.

We demonstrated that thin films BFO produced by sol-gel process exhibit in the state where polarization is oriented preliminary in one crystallographic direction (Figure 1). This is not correlated with tetragonal symmetry reveled by X-ray. Such a polarization “self-orientation” could be occurred at the stage of the thin film crystallization and leads to the formation of the cluster-like domain structure where the preliminary single domain areas are confined in the clusters with average size about 500 nm – 1 μm consisted of 10-20 grains. The boundaries of the clusters possesses enhanced conductivity one order higher the bulk. The polarization switching does not change the position of the conductive boundaries, which could be a sign that they were built-in at the stage of film crystallization.

Analysis of BFO ceramics doped with Sm with the composition near the morphotropic phase boundaries by X-ray diffraction and piezoresponse force microscopy reveled structural state with coexistence anti-polar and polar phase. The phase boundaries between polar and non-polar phase and domain walls have a conductivity significantly higher the bulk, which we addressed to their charge state. We showed possibility to modify the phase of the material using controllable action of the electric field inducing phase transition anti-polar to polar phase localized near the scanning probe microscopy tip. The formed state was stable for a long period (above 2 days).

The experiments with phase boundaries and domain walls in BFO suggests new ways for the enhancement of the macroscopic properties of the materials using domain wall and phase interface engineering.

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